



Parameters fitting of soil hydraulic functions: Lognormal pore size distribution in bi-modal soils

L. Jendele (1,3), and M. Kutílek (2)

(1) Cervenka Consulting, Prague, Czech Republic, (2) Emeritus professor Czech Technical University, Prague, Czech Republic, (3) libor.jendele@atlas.cz

Soil water saturation curve and saturated/unsaturated hydraulic conductivity are important soil characteristics for transport processes in soils and their accurate numerical modeling is crucial for any high quality computer simulation. This paper presents a procedure for parameter fitting for a constitutive model based on lognormal pore size distribution (see (Kosugi 1996; Kosugi 1999) used for bi-modal soils (Kutílek 2004). The model was successfully used for several soil types (Kutílek et al. 2005, Kutílek and Jendele 2005). Based on the present procedure a computer program was developed that automates the whole process of the parameters' optimization.

The constitutive model is based on the following two equations:

$$S_i = \frac{1}{2} \operatorname{erfc} \left[\frac{\ln(h_i/h_{mi})}{\sigma_i \sqrt{2}} \right] \quad (1)$$

$$K_{Ri} = S_i^{\alpha_i} \left\{ \frac{1}{2} \operatorname{erfc} \left[\left(\ln \frac{h_i}{h_{mi}} \right) \frac{1}{\sigma_i \sqrt{2}} + \frac{\beta_i \sigma_i}{\sqrt{2}} \right] \right\}^{\gamma_i} \quad (2)$$

Equation (1) predicts degree of effective soil saturation S_i as a function of hydraulic head of capillary pressure h_i , whilst Equation (2) is used to calculate relative hydraulic conductivity of soil phase K_{Ri} . The remaining parameters have to be fitted.

As the present model is for bi-modal soils, the above equations are written for matrix pores, ($i = 1$) and structural pores, ($i = 2$). Thus, we have to find an optimal value for the parameters h_{m1} , h_{m2} , σ_1 , σ_2 , α_1 , β_1 , γ_1 , α_2 , β_2 , γ_2 . This is not an easy task, because Equations (1) and (2) are highly nonlinear. The proposed fitting procedure is iterative and includes steps for graphical visualization of measured and computed data

on the soil saturation and hydraulic conductivity. They assist the engineer to assess accuracy of the computed approximations.

The process of the parameters fitting consists of several steps. They are now described for the case of the parameters h_{m1} , h_{m2} , σ_1 , σ_2 .

1. Read data on measured soil water content θ , i.e. k data pairs (θ_k, h_k) .
2. Calculate residual and saturated volumetric water content θ_r , θ_s and calculate soil effective saturation S_k , (in all the k points).
3. Create a piecewise polynomial interpolation of S as a function of $\ln(h)$ that passes thru the points S_k . If only continuity of S is requested, (near all k points), each of the interpolated $k-1$ interval of S can be approximated linearly. Otherwise, nonlinear approximation is needed and it would ensure also continuity of $dS/d(\ln(h))$.
4. Using the above approximation generate a larger data set of $(S_j, \ln(h_j))$, $j = 1..m$, where m is typically about 200 points. Generate the similar set for $dS/d(\ln(h))$. Draw the above sets.
5. Set value of h_a , i.e. a capillary pressure separating matrix and structural pores. This value is indicated by a peak in $dS/d(\ln(h))$, (see Kutilek, 2004). Calculate θ_{s1} , which is saturated volumetric index for matrix domain.
6. Based on θ_{s1} calculate pore and matrix saturations S_1, S_2 in m points and compute the first approximation of the parameters h_{m1} , h_{m2} , σ_1 , σ_2 . Because of similarity between lognormal distribution function of soil radius and (\cdot) , these are mean value and standard deviation of the calculated S_1, S_2 distribution functions.
7. Use conjugate gradient method (Powell 1977; Powell 1978) to optimize the approximation of S by (\cdot) . Note that $S_1 + S_2$ is compared against measured S_j . This yields new values for h_{m1} , h_{m2} , σ_1 , σ_2 . Optionally, the value of h_a can also be subject of the optimization process, however our experience shows that manual setting of h_a by an experienced engineer usually ensures better results.
8. Draw the approximated and measured function S to allow for visual accuracy assessment. If the approximation is successful, proceed to the approximation of relative hydraulic conductivity. Otherwise, change the value of h_a , m and other input parameters to improve accuracy of the current approximation.

In the next phase, carry on similar procedure to optimize the parameters $\alpha_1, \beta_1, \gamma_1, \alpha_2, \beta_2, \gamma_2$. However, as it was found that the same quality approximation can be obtained for the whole range of values of γ_1, γ_2 , we assume $\gamma_1 = \gamma_2 = 1$ in our work. In addition to simplifying the optimization process itself, this assumption also significantly simplifies use of the constitutive law during subsequent transport analyses.

Note that in the case of optimizing $\alpha_1, \beta_1, \alpha_2, \beta_2$ we don't have a good guess approximation similar to add.6. Hence, good starting values for the parameters are obtained simply by scanning the space of $\alpha_i \in \langle -2..3 \rangle, \beta_i \in \langle 0.1..4 \rangle$ (in many equally distributed points) for the best fit of (). Thereafter, the conjugate gradient optimization is executed in similar way to that described for the parameters $h_{m1}, h_{m2}, \sigma_1, \sigma_2$. Note also that during the fitting it is sometimes advantages to minimize relative error (rather than absolute error) of Equation ().

The described procedure proves robust and efficient. It converges within few seconds, thereby it enables use of relatively complex constitutive model based in (), () for bi-modal soils.

Keywords: Pore size distribution; Bi-modal soils; Structural porosity; Matrix porosity; Soil water retention; Numerical modeling; Numerical simulation.

Acknowledgements This research was supported by the Czech Grant Agency, grant GACR No. 103/05/2143.

References:

- Kosugi, K. (1996). Lognormal distribution model for unsaturated soil hydraulic properties. *Water Resources Res.* 32(9): 2697-2703.
- Kosugi, K. (1999). General model for unsaturated hydraulic conductivity for soils with lognormal pore-size distribution. *Soil Sci. Soc. Am. J.* 63(??): 270-277.
- Kutilek, M. (2004). Soil hydraulic properties as related to soil structure. *Soil Tillage Res.* 79: 175-184.
- Kutilek, M., Jendele, L., and Panayiotopoulos, K.P. (2005). The influence of uniaxial compression upon pore size distribution in bi-modal soils. Accepted for publication, *Soil Tillage Res.*
- Kutilek, M., and Jendele, L. (2005). Lognormal pore size distribution in bi-modal soils: Hydraulic functions. Submitted to *Soil Sci. Soc. Am. J.*
- Powell, M. J. D. (1977). Restart procedures for the conjugate gradient method. *Mathematical Programming* 12: 241-254.

Powell, M. J. D. (1978). A Fast Algorithm for Nonlinearly Constrained Optimization Calculations. Numerical Analysis Proceedings, Dundee, Springer-Verlag.